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# Effects of the constriction geometry on quasi-one-dimensional transport: Adiabatic evolution and resonant tunneling

E. Tekman and S. Ciraci
*Department of Physics, Bilkent University, Bilkent 06533, Ankara, Turkey*
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The geometry of a constriction, which plays a crucial role in quasi-one-dimensional (quasi-1D) ballistic transport, is investigated by performing calculations of the conductance. If the constriction becomes smoothly narrower inside, the current-carrying states evolve adiabatically leading to quantized conductance without a resonance structure. In contrast, quasi-0D (confined) states can form in a local widening inside the constriction and give rise to resonant tunneling. The effects of an obstacle at the entrance and the roughening along the constriction are also studied.

The effects of the quantization of the transverse momentum in infinite one-dimensional (1D) electron waveguides were investigated theoretically,[1] and the conductance of this constriction $G_c$ was predicted to be quantized as the multiples of $2e^2/h$. Recently, van Wees *et al.*[2] and Wharam *et al.*[3] measured the conductance through a constriction between two 2D electron-gas (EG) reservoirs. They found that in compliance with the earlier theory,[1] the conductance increases with the gate voltage $V_g$ (or equivalently with the width $w$ of the constriction) approximately in steps of $2e^2/h$. This experimental observation of the step structure in the conductance has attracted a lot of interest. Several theories[4-8] have been developed with the assumption that the transport is ballistic, as pointed out by the experimentalists,[2,3] and the emphasis has been placed on the critical effect of the boundaries between the 2D EG and the constriction. In fact, reflections of the electron waves from the boundaries were shown to result in the resonance structure on the plateaus.[4-8] While the lack of the resonance structure in the experiments was attributed to the finite-temperature effects[5,8] or to scattering from the nonuniform constriction potential,[6,9] García objected to the ballisticity of the transport.[10] In the meantime, the measurements on two consecutive constrictions separated by an electron gas yielding only $G$ corresponding to the narrower one[11] have been taken as evidence for the ballisticity of the transport.

Earlier, we presented a refined formalism[8,9] of the quantum conductance through a constriction and provided the exact calculation of $G$. In the formalism the current-carrying states are obtained by the boundary matching of the plane-wave states in the 2D EG to the states which are quantized in the constriction. The spatial form of the potential, $V(y,z)$, of the constriction depends on the gate voltage, as such that it is parabolic for small $w$ (large $-V_g$), but becomes square-well-like at large $w$ (small $-V_g$).[12] We considered an infinite well potential, since in the energy range relevant to the experiments it yields eigenstates similar to that of the square well, but provides a substantial convenience in computations. Nevertheless, the form of the potential influences the spacings of the steps in the $G(w)$ curve, but the underlying physics essentially remains unaltered.

The expression we obtained for the conductance is given in matrix form:[8,9]

$$G=\frac{e^2}{\pi h}\int_{-k_F}^{k_F}\frac{d\kappa}{k_z(\kappa)}\{[\tilde{\Theta}^\dagger(\mathbf{k})\tilde{\Gamma}_R\tilde{\Theta}(\mathbf{k})-\tilde{\Delta}^\dagger(\mathbf{k})\tilde{\Gamma}_R\tilde{\Delta}(\mathbf{k})] +2\,\mathrm{Im}[\tilde{\Theta}^\dagger(\mathbf{k})\tilde{\Gamma}_I\tilde{\Delta}(\mathbf{k})]\}\,. \quad (1)$$

$\tilde{\Theta}(\mathbf{k})=[\tilde{\mathrm{I}}-(\tilde{\mathrm{r}}e^{i\tilde{\Gamma}d})^2]^{-1}\tilde{\mathrm{t}}_\mathbf{k}$ and $\tilde{\Delta}(\mathbf{k})=e^{i\tilde{\Gamma}d}\tilde{\mathrm{r}}e^{i\tilde{\Gamma}d}\Theta(\mathbf{k})$ are expressed in terms of the reflection matrix $\tilde{\mathrm{r}}$ and the transmission vector $\tilde{\mathrm{t}}_\mathbf{k}$ which are analogous to the reflection and transmission coefficients for a 1D step potential. The diagonal matrix $\tilde{\Gamma}$ has elements $(\Gamma_{ij})^2=\delta_{ij}2m^*(E-\varepsilon_n)/\hbar^2$ for energy $E$, with the effective mass $m^*$ and constriction eigenenergy $\varepsilon_n$, and is expressed as $\tilde{\Gamma}=\tilde{\Gamma}_R+i\tilde{\Gamma}_I$. In the expression of conductance, the interference effects of the reflected waves are built in by the separation of the right-going (first term) and left-going (second term) states. The evanescent states in the third term contribute as tunneling, and smooths out the sharp rises in $G$ corresponding to the opening of a new channel. This effect becomes significant at small constriction length $d$. As pointed out earlier,[8] for the simplest system that is a uniform quasi-1D constriction between two 2D EG, the quantization of $G$ starts at $d\simeq\lambda_F$ and steps occur exactly at the integer multiples of $2e^2/h$ only for $d\gtrsim 5\lambda_F$. The case of $d=0$ corresponds to Sharvin conductance,[13] $G_s=(2e^2/h)2w/\lambda_F$, but the whole curve is displaced and weak oscillations are superimposed owing to the quantum interference effects. However, the larger $d$ is, the sharper the quantum jumps are, and the flatter the plateaus are. In addition, the resonance structure, which originates from the interference of multiple reflected waves, superimposed on the flat plateaus, becomes more pronounced at large $d$.

The resonance structure is the crucial aspect of the ballistic transport through a quasi-1D constriction. It has to appear only when the phase coherence is maintained during the transport, but can be destroyed due to the elastic scattering and Fermi-level smearing at finite temperature,[8] or due to the inelastic scattering. Nonuniform constrictions, tapering, surface roughness, and the impurities in the constriction may lead to elastic scattering, in which the resonance structure may get weaker due to the mixed phases of the wave functions. If the transport is really ballistic as is presumed, the phase incoherence due to elastic scattering or finite temperature may explain why the observed $G(V_g)$ curves are lacking the resonance structure. Clearly, the geometry of the constriction has important implications, and is essential for a thorough understanding of the 1D transport. The effect of the self-consistent potential—which happens to deviate from the square-well or parabolic potential used in the calculations—can also be deduced to some extent from the study of the constriction geometry.

In this paper, we investigate the effects of the constriction geometry on the conductance. The major advantage of the formalism[8] outlined above lies in its extension to various geometries. In this case the constriction is described by closely spaced uniform constrictions with different widths, and a transfer-matrix method is used for multiple boundary matching. We found that for a tapered constriction of uniform length $d_0 \sim \lambda_F$ the plateaus do not reach to the quantized values if the tapering angle $\alpha < 75°$. In contrast, for the large tapering angle $\alpha > 85°$ (i.e., small deviation from the uniformity) the wave function can evolve adiabatically with depressed scattering. As a result, steps become sharp and the plateaus are flat, but the resonance structure is destroyed to a large extent. In the rough constriction, the heights of the steps deviate from the ideal value of $2e^2/h$ and the resonance structure is distorted and becomes either weaker or stronger. For the first time, we show that a local widening of the constriction may lead to quasi-0D states, which in turn gives rise to resonant tunneling.

In Fig. 1, we present the $G(w)$ curves calculated for various tapered constrictions. As described in the inset, the length of the uniform part is $d_0$, and the tapering is characterized by $d$ and $\alpha$. For the case of $d_0 = 0$, $G$ exhibits a behavior reminiscent of the Sharvin conductance even for $\alpha \sim 45°$. As $\alpha$ increases the oscillations develop and change into the step structure. By the inclusion of a uniform constriction of $d_0 = \lambda_F$ between two taperings the conductance changes. The steplike structure appears even for $\alpha = 45°$. Although the plateaus cannot be flattened, and thus cannot reach the quantized values, a resonance structure which is seen in the abrupt and uniform constriction of $d_0 = \lambda_F$ (i.e., $d = 0$) is maintained for $\alpha \lesssim 85°$. However, as in the previous cases for $\alpha \gtrsim 85°$ the resonance structure disappears to yield a well-defined step structure. Contrary to this situation, one would expect pronounced and sharper resonance structure since the tapering changes into the uniform constriction as $\alpha \rightarrow 90°$, and thus its length increases from $d_0$ to $d_0 + 2d$.

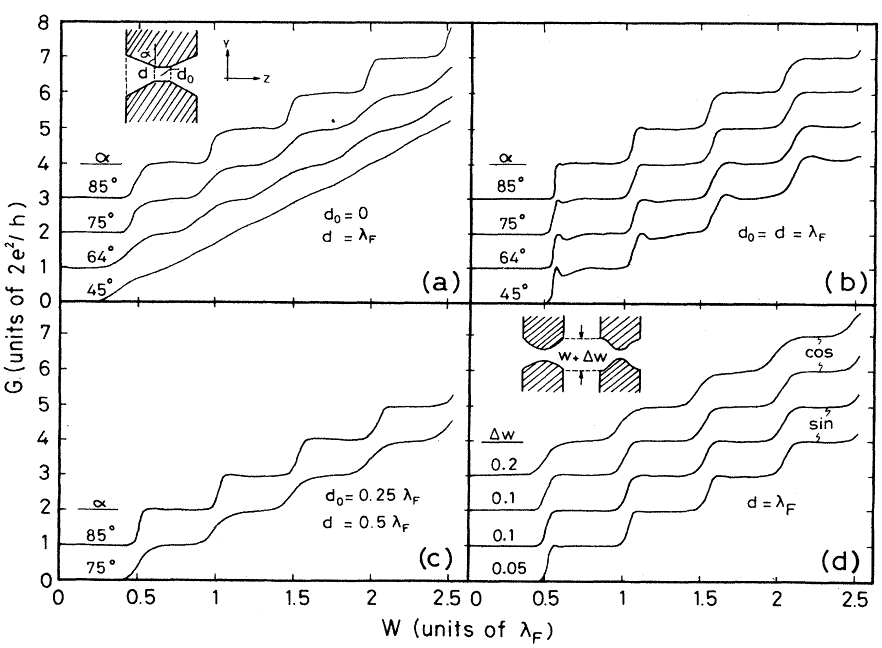


FIG. 1. Calculated $G(w)$ curves showing the adiabatic evolution of the constriction states for certain geometries. (a)–(c) correspond to tapering with different parameters described by the inset in (a). In (d) the constriction is modulated by sine- and cosine-profiles.

This behavior of $G$ is related to the adiabatic evolution of the current-carrying wave. Since $|\partial w/\partial z|$ is small for large $\alpha$, a state entering the tapering evolves without changing the quantum number $n$ associated with the $y$ momentum, while the energy $\varepsilon_n(z)$ and the momentum $k_y$ increase. The conditions, in which the adiabatic evolution of the states takes place, depend on the geometry of the constriction. It appears that a tapering with $\alpha \simeq 85°$ satisfies this condition. Because of the adiabatic evolution, the quantization of conductance is not affected in any essential manner,[14,15] but owing to the insufficient phase coherence the resonance structure disappeared. A similar behavior was shown to exist for a constriction between two large circles.[14] The constriction described in Fig. 1(d) mimics that geometry, where the widths $w$ are given by $w(z) = w + \Delta w(1 - \sin(\pi z/\lambda_F))$ and $w(z) = w + \frac{1}{2}\Delta w(1 - \cos(2\pi z/\lambda_F))$ for amplitude $\Delta w$ ranging from 0.05 to 0.2 $\lambda_F$. While adiabatic evolution is complete for small $\Delta w$ and yields sharp steps and almost flat plateaus, the steps are not as sharp for large $\Delta w$.

Contrary to the above geometry, a finite constriction which is relatively narrower at both ends gives rise to the spatially varying subband energies, $\varepsilon_n(z)$, which are lowered near the center of the constriction. As schematically described in Fig. 2(a) these subbands can be viewed as the potential wells,[16] in which quasi 0D (or confined) states are formed. A similar confinement can occur even if the widening is abrupt inside the constriction. This situation is reminiscent of a double-barrier resonant tunneling (DBRT) structure, and hence may lead to the resonant tunneling. Before the $n$th channel ($n \geq 1$) is opened, the resonance may occur on the $(n-1)$th plateau whenever a confined state in the well of $\varepsilon_n(z)$ matches to the states of the 2D EG. As a result, resonance peaks illustrated in Fig. 2(b) appear near the edges of the quantum steps of $G(w)$.

We used sine and cosine modulation along the constriction with the amplitude $\Delta w$. We found that the sine modulation yields relatively smaller widths $w_r$ (at which resonant tunneling occurs), and broader peaks as compared to those of the cosine modulation. This can be explained by using the DBRT analogy. Since the sine modulation is represented by a DBRT structure with a relatively wider well, but narrower barriers as compared to those of the cosine modulation, the resonance energies are relatively farther from the top of the barrier (or equivalently from the quantized steps in $G$) and resonance peaks are relatively broader for the sine modulation. That the DBRT analogy is valid and thus the peaks near the steps are related to the resonant tunneling are shown by calculating the quasi-0D states for an infinite constriction with a widening of the same form as the finite constriction above and by comparing the positions of these with the resonance positions $w_r$.

Next we investigate the effect of the roughness along the constriction, which is closely related to the quality of the split gate. As shown in the inset of Fig. 3, the roughness is simulated by a random modulation of the width. At each step, $\delta d = d/N$ along the constriction $w$ is varied by $x\Delta w$, where the value of $x (0 \leq x \leq 1)$ is random. This

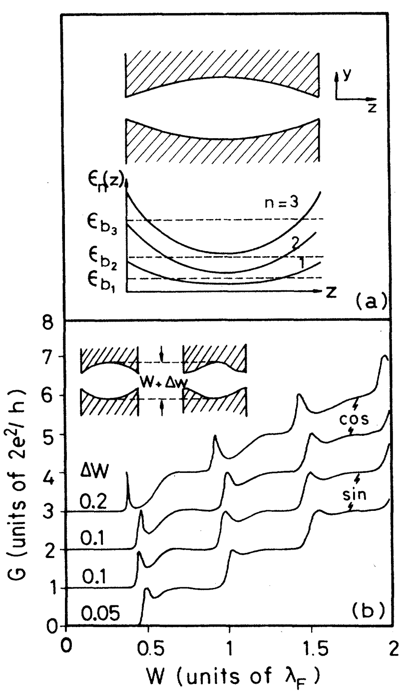


FIG. 2. (a) A schematic description for the formation of the quasi 0D states ($\varepsilon_b$) in a constriction. (b) $G(w)$ calculated for constrictions modulated by sine- and cosine-profiles.

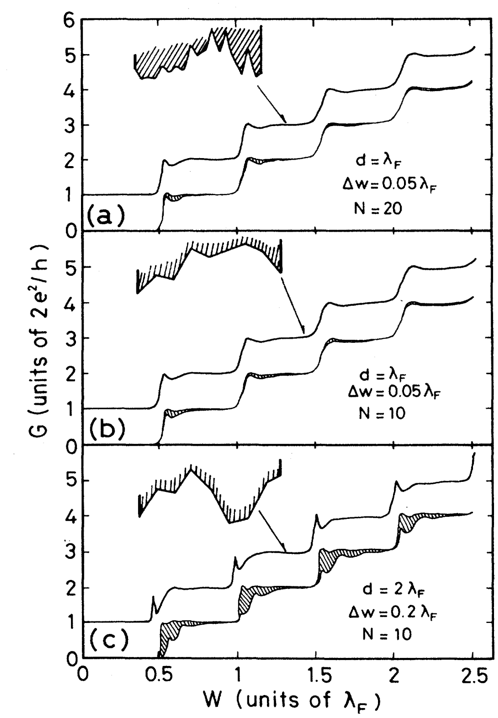


FIG. 3. In each panel a single $G(w)$ curve calculated for a specific profile $w + \delta w(z)$ (shaded line in upper left-hand side) reproducing a rough constriction. Shaded plot is generated from 25 $G(w_{av})$ curves calculated for different, randomly selected profiles.

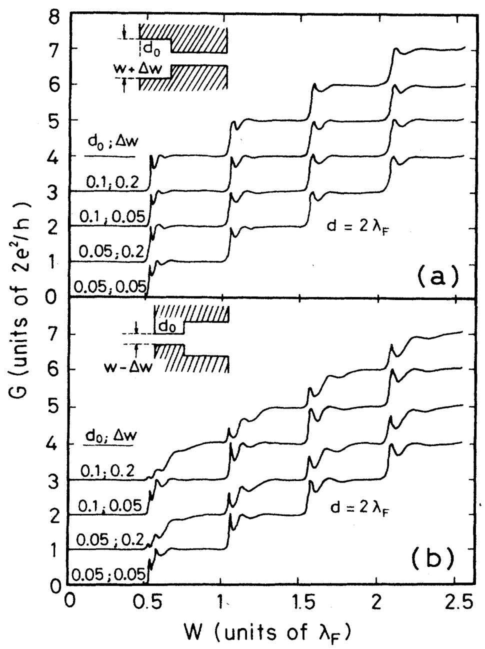


FIG. 4. $G(w)$ curves calculated for an obstacle at the entrance of a uniform constriction.

way a histogram profile $\delta w(z)$ is superimposed over the uniform width $w$. The $G(w)$ is then calculated for 25 different $\delta w(z)$ profiles, and is traced on the same plot with respect to the average width

$$w_{av}=w+d^{-1}\int_0^d \delta w(z)dz\ .$$

The conductance $G(w_{av})$ for a given set of $(d,\Delta w)$ varies in the shaded region as a function of the profile. The width of the shaded region increases with increasing $\Delta w$. In each panel in Fig. 3 $G(w)$ is also presented corresponding to a specific profile. Since $\Delta w$ is small, the positions of the resonance peaks are maintained. Nevertheless, the conductance values at the resonances and antiresonances are affected because of the scattering from the roughness.

Finally, we discuss two forms of the constriction described in Fig. 4. These are obtained by implementing an obstacle of length $d_0$ at the entrance of a uniform constriction of length $d$. The width of the obstacle is relatively larger or smaller ($\pm\Delta w$). In the first one, since the states in the obstacle region can match the 2D EG states to those of the uniform constriction, the conductance is not affected. In contrast, the narrower obstacle lacks appropriate states, which match the uniform constriction to the 2D EG. Since the openings of the channels are shifted to $n\lambda_F/2+\Delta w$, the sharp step structure is disturbed and the flat plateaus disappear with increasing $\Delta w$. We notice that even for $d_0=0.05\lambda_F$ a small reduction of $w$ at the entrance gives rise to drastic deviations from the ideal $G(w)$ curve of the uniform constriction. If such an obstacle is put in the constriction near the center, its effect is not as drastic as the previous one.

In conclusion, we showed that the form of the constriction plays an essential role in the measured conductance $G(w)$ for the 1D ballistic transport between two 2D EG reservoirs. If the variation of $w(z)$ is very small and smooth, permitting adiabatic evolution of the wave function, the quantized conductance with step structure is maintained, but the resonance structure disappears. We predict that the resonant tunneling may occur in a constriction which becomes relatively wider at the center.

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